Quantum Mechanics 2
Spring 2019

Midterm 1 Solutions

1. A spinless particle is described by the Hamiltonian:

$$H = \frac{p^2}{2m} + \alpha(x^2 + y^2 + z^2) \tag{1}$$

Determine two symmetry operators that H remains invariant under.

Answer: H is invariant under all rotations in 3 dimensions, reflections (parity), and time translations. Rotations and reflections can be seen from the fact that the momentum and position vector operators transform under rotations and reflections in exactly the same way that regular 3-vectors transform under these symmetries. Since the Hamiltonian is built from the magnitudes of the momentum and position operators which are manifestly rotationally (and parity) invariant, the Hamiltonian itself is invariant. Also, time translations are of course a symmetry because they are generated by the Hamiltonian and the Hamiltonian commutes with itself. Any Hamiltonian depending on only position and momentum without explicit time dependence is invariant under time translation symmetry.

2. Derive the first order corrections to the energy levels in non-degenerate perturbation theory for Hamiltonian $H = H_0 + \lambda H'$ where the unperturbed Hamiltonian has distinct energy levels E_n^0 and eigenfunctions ψ_n^0.

Solution: The first step in perturbation theory is assume that the exact energy levels E_n and eigenfunctions ψ_n can be expanded in a Taylor series in λ:

$$\begin{aligned} E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \\ \psi_n &= \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots \end{aligned} \tag{2}$$

and then the goal is to compute these terms in the series order by order with the hope that the series converges to the exact solution so that if we cut off the series at some order in λ, the partial sum can rightly be said to approximate the exact solutions. Now we right down the eigenvalue problem $H\psi_n = E_n\psi_n$

$$(H_0 + \lambda H')(\psi_n^0 + \lambda\psi_n^1 + \dots) = (E_n^0 + \lambda E_n^1 + \dots)(\psi_n^0 + \lambda\psi_n^1 + \dots) \tag{3}$$

Keeping only the first order terms, we have:

$$H_0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0 \tag{4}$$

If we take the inner product with $\psi_n^{0\dagger}$, we get:

$$\psi_n^{0\dagger}H_0\psi_n^1 + \psi_n^{0\dagger}H'\psi_n^0 = E_n^0\psi_n^{0\dagger}\psi_n^1 + E_n^1\psi_n^{0\dagger}\psi_n^0 \tag{5}$$

Now since H_0 is Hermitian, we know $\psi_n^{0\dagger}H_0 = \psi_n^{0\dagger}E_n^0$. Therefore, the first terms on the left and right cancel. Furthermore, since ψ_n^0 has norm one, the remaining term on the right is just E_n^1 giving us the first order corrections to the energy levels as:

$$E_n^1 = \psi_n^{0\dagger}H'\psi_n^0 \tag{6}$$

3. Consider a free electron in the spin state $|\uparrow\rangle$ (with magnetic moment $\vec{\mu} = -\frac{e}{m}\vec{S}$) in the presence of a strong magnetic field $\vec{B} = B_z\hat{z}$. The Hamiltonian due to the field is $H_0 = -\mu_z B_z$. Suppose that a small additional magnetic field $B_x\hat{x}$ is imposed. What is the change to the electron energy to: (a) First order in perturbation theory (b) to second order in perturbation theory

   (a) First Order

Solution: Recall that spin-$\frac{1}{2}$ operator is given by $S_i\frac{\hbar}{2}\sigma_i$ where σ_i are the Pauli matrices ($\sigma_1 = \sigma_x, \sigma_2 = \sigma_y, \sigma_3 = \sigma_z$. Therefore, the unperturbed Hamiltonian is $H_0 = \frac{\hbar e B_z}{2m}\sigma_z$. It's eigenstates are $|\uparrow\rangle, |\downarrow\rangle$ with energies $E^0_\uparrow = -E_\downarrow = \frac{\hbar e B_z}{2m}$. The perturbation is $H' = \frac{\hbar e B_x}{2m}\sigma_x$. We wish to find the first order correction to the state $|\uparrow\rangle$. The correction is $\langle\uparrow|H'|\uparrow\rangle = \frac{\hbar e B_x}{2m}\langle\uparrow|\sigma_x|\uparrow\rangle$. However, we know $\sigma_x|\uparrow\rangle = |\downarrow\rangle$ and $\langle\uparrow|\downarrow\rangle = 0$. Therefore, $E^1_\uparrow = 0$.

(b) Second Order

Solution: Recall the general formula for second order corrections:

$$E^2_n = \sum_{m\neq n} \frac{|\langle m|H'|n\rangle|^2}{E^0_n - E^0_m} \tag{7}$$

In our case, the state "n" is $\uparrow$ and the only state that is not $\uparrow$ is $\downarrow$. Therefore the only m in the sum is $\downarrow$ and we get:

$$E^2_\uparrow = \frac{|\langle\downarrow|H'|\uparrow\rangle|^2}{E^0_\uparrow - E^0_\downarrow} \tag{8}$$

Recalling our formula for the unperturbed energies mentioned in (a), we know $E^0_\uparrow - E^0_\downarrow = \frac{\hbar e B_z}{m}$. If we also factor out $\frac{\hbar e B_x}{2m}$ from H', we get:

$$E^2_\uparrow = \frac{\left(\frac{\hbar e B_x}{2m}\right)^2 |\langle\downarrow|\sigma_x|\uparrow\rangle|^2}{\left(\frac{\hbar e B_z}{m}\right)} \tag{9}$$

We already know $\sigma_x|\uparrow\rangle = |\downarrow\rangle$ and $\langle\downarrow|\downarrow\rangle = 1$. Therefore, canceling a few factors on the numerator and denominator, we get:

$$E^2_\uparrow = \frac{\hbar e B_x^2}{4mB_z} \tag{10}$$

4. Consider a 3D infinite square well with sides of length a to which we add the following perturbation:

$$H'(x,y,z) = \{ \begin{array}{cc} V_0 & 0 < x, y < a \\ 0 & \text{otherwise} \end{array} \tag{11}$$

Apply degenerate perturbation theory and find the corrections to the energies. For reference, the 1D wave functions and energies are:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}) \tag{12}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{13}$$

Solution: A basis of energy eigenfunctions for the unperturbed square well along with their energies are the following:

$$\psi_{n_1,n_2,n_3}(x,y,z) = \psi_{n_1}(x)\psi_{n_2}(y)\psi_{n_3}(z) \tag{14}$$

$$E_{n_1,n_2,n_3} = (n_1^2 + n_2^2 + n_3^2)\frac{\pi^2\hbar^2}{2ma^2} \tag{15}$$

The ground state is of course $\psi_{1,1,1}$ and the three degenerate first excited states are $\psi_{2,1,1}, \psi_{1,2,1}, \psi_{1,1,2}$. For notational simplicity, let us denote these 3 states as $\psi_{2,1,1} = |1\rangle, \psi_{1,2,1} = |2\rangle, \psi_{1,1,2} = |3\rangle$. Our goal then is to determine the matrix $V_{ij} = \langle i|H'|j\rangle$ for $i, j = 1, 2, 3$ and then find it's eigenvalues which will give us the first order corrections. A general matrix element of H' can be written as:

$$\begin{aligned}\langle\psi_{n_1,n_2,n_3}|H'|\psi_{m_1,m_2,m_3}\rangle &= \int_0^a dx \int_0^a dy \int_0^a dz \psi_{n_1,n_2,n_3}(x,y,z)^* H'(x,y,z)\psi_{m_1,m_2,m_3}(x,y,z) \\ &= V_0\Big(\int_0^{\frac{a}{2}} dx\psi_{n_1}^*\psi_{m_1}\Big)\Big(\int_0^{\frac{a}{2}} dy\psi_{n_2}^*\psi_{m_2}\Big)\Big(\int_0^a dz\psi_{n_3}^*\psi_{m_3}\Big)\end{aligned} \tag{16}$$

We will first compute the diagonal elements V_{ii}. Then we will compute the off-diagonal elements V_{i3}. And finally, we will compute V_{12}. If the entries are diagonal in (16), then the first two terms in parenthesis are integrating a norm one function over half of the space giving $\frac{1}{2}$ and the third term is integrating a norm one function over the whole space giving 1. Therefore, the diagonal entries are

$$V_{ii} = \frac{V_0}{4} \tag{17}$$

Next, for the off-diagonal terms of the form V_{i3}, the third factor in parenthesis in (16) would be taking the inner product of ψ_3 with ψ_i for $i \neq 3$ which gives 0 because the 1D basis is orthogonal.

Finally, the entry V_{12}. Let us write it explicitly:

$$V_{12} = V_0 \Big(\int_0^{\frac{a}{2}} dx \psi_2^* \psi_1 \Big) \Big(\int_0^{\frac{a}{2}} dy \psi_1^* \psi_2 \Big) \Big(\int_0^{a} dz \psi_1^* \psi_1 \Big) \tag{18}$$

The last factor is just 1 and the first two factors are the same. Therefore we just need to compute one of those factors. We do so as follows:

$$\begin{aligned} \int_0^{\frac{a}{2}} dx \psi_2^*(x) \psi_1(x) &= \frac{2}{a} \int_0^{\frac{a}{2}} dx \, \sin(\frac{2\pi x}{a}) \, \sin(\frac{\pi x}{a}) \\ &= \frac{2}{\pi} \int_0^{\frac{\pi}{2}} du \, \sin(2u) \, \sin(u) \\ &= \frac{4}{\pi} \int_0^{\frac{\pi}{2}} du \, \cos(u) \, \sin(u)^2 \\ &= \frac{4}{\pi} \int_0^{1} dv v^2 \\ &= \frac{4}{3\pi} \end{aligned} \tag{19}$$

In the second line, we used the substitution $u = \frac{\pi x}{a}$. In the third line, we used the identity $\sin(2u) = 2 \sin(u) \cos(u)$. In the fourth line, we used another substitution $v = \sin(u)$. Plugging this result back into (18), we get:

$$V_{12} = \frac{16V_0}{9\pi^2} \tag{20}$$

Putting everything together, our matrix V_{ij} is:

$$V = \begin{pmatrix} \frac{V_0}{4} & \frac{16V_0}{9\pi^2} & 0 \\ \frac{16V_0}{9\pi^2} & \frac{V_0}{4} & 0 \\ 0 & 0 & \frac{V_0}{4} \end{pmatrix}.$$

To find the eigenvalues, we must solve the characteristic equation:

$$(\lambda - \frac{V_0}{4})((\lambda - \frac{V_0}{4})^2 - \left(\frac{16V_0}{9\pi^2}\right)^2) = 0 \tag{21}$$

The solutions (and thus the first order corrections to the eigenvalues) are:

$$\lambda = \frac{V_0}{4}, \frac{V_0}{4} \pm \frac{16V_0}{9\pi^2} \tag{22}$$